

(¹³C₃)Propan-2-ol
220505-06-6 | DTXSID10745773

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 2.58e-01

Global applicability domain: Inside

Local applicability domain index: 6.45e-01

Confidence level: 7.38e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Isopropanol</div> <div>Measured: 0.05</div> <div>Predicted: 2.58e-01</div>	<div>Image not found</div> <div>1-Propanol</div> <div>Measured: 0.25</div> <div>Predicted: 1.27e-01</div>	<div>Image not found</div> <div>2-Butanol</div> <div>Measured: 0.61</div> <div>Predicted: 7.73e-01</div>
<div>Image not found</div> <div>1-Butanol</div> <div>Measured: 0.88</div> <div>Predicted: 8.38e-01</div>	<div>Image not found</div> <div>2-Methyl-1-propanol</div> <div>Measured: 0.76</div> <div>Predicted: 8.81e-01</div>	